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Ground State Wave Functions in the Hyperspherical Formalism for Nuclei with $A > 4$

Nir Barnea¹⁾, Winfried Leidemann^{2,3)}, and Giuseppina Orlandini^{2,3)}

1) European Centre for Theoretical Nuclear Physics and Related Areas, Villa Tambosi, I-38050
Villazzano (Trento), Italy

2) Dipartimento di Fisica, Università di Trento, I-38050 Povo (Trento), Italy

3) Istituto Nazionale di Fisica Nucleare, Gruppo collegato di Trento, Italy

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Abstract

The general formulation of a technically advantageous method to find the ground state solution of the Schrödinger equation in configuration space for systems with a number of particles A greater than 4 is presented. The wave function is expanded in pair correlated hyperspherical harmonics beyond the lowest order approximation and then calculated in the Faddeev approach. A recent efficient recursive method to construct antisymmetric A -particle hyperspherical harmonics is used. The accuracy is tested for the bound state energies of nuclei with $A = 6 \div 12$. The high quality of the obtained results becomes evident from a comparison with other approaches.

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I. INTRODUCTION

Few–body nuclei with a number of nucleons A between 5 and 16 are a particularly interesting testground for nuclear theory. They lie in the range between the classical few–nucleon systems ($A \leq 4$) and the smallest nuclei, which can be described realistically starting from a mean field ansatz. Therefore one hopes that these nuclei could build a link between few–body and many–body physics. Presently quite an effort is made for a better understanding of these intermediate systems. Specific interest is devoted to halo–nuclei, but also the less exotic nuclei of this mass range are investigated thoroughly. Many theoretical techniques for the calculation of their ground states have been imported from the classical few–body field, where there has been a considerable progress in the last years. In fact for the classical few–body systems rather different approaches have been developed and proven to lead to precise results. These methods include solutions of the Faddeev–Yakubovsky equation, variational (VMC) and Green Function Monte Carlo (GFMC), the Hyperspherical Harmonic (HH) ansatz, the stochastic variational (SVM), as well as coupled cluster and resonating group methods.

For nuclei with $A > 4$ a similar level of precision has not yet been reached. Here GFMC has led to the most accurate results. Exact bound state energies with realistic NN interactions have been calculated for $A \leq 9$ [1]. Unfortunately wave functions cannot be generated with this method. Recently, a very powerful tool to calculate few–body wave functions has been developed with the SVM ansatz [2,3]. However, this approach is probably most suitable for systems with $A < 8$. For nuclei with $A \geq 8$ rather good results have been obtained in the Integro–Differential Equation Approach (IDEA) [4], which uses the HH expansion at first order, and with a variational method, the Translational Invariant Configuration Interaction Method (TICI) [5,6], which is inspired by the coupled cluster method.

In this work we present the general formulation of the method, which combining the main ideas of the HH expansion, the pair correlation ansatz and the Faddeev approach allows to calculate wave functions of few–body systems. We apply it to calculate the binding energies of nuclear systems with 6, 8 and 12 particles. Including higher order HH functions we make the nontrivial step beyond the IDEA approach. The difficulty in constructing antisymmetric A –particle HH is overcome by the use of a recently developed very efficient recursive method [7], where HH basis functions are constructed, belonging to well defined irreducible representations of the orthogonal and symmetric groups.

The paper is organized as follows. The method is described in Section II, while the construction of the HH basis function is briefly reviewed in Section III. Section IV illustrates how the matrix elements are calculated and the obtained results for the binding energies of nuclei with $A = 6, 8$ and 12 are discussed in Section V. Conclusions are drawn in Section VI.

II. GENERAL FORMULATION OF THE METHOD

Our aim is the solution of the Schrödinger equation for a system of A particles interacting via a two–body potential. After subtraction of the center of mass Hamiltonian the problem

reduces to the solution of the internal Hamiltonian in terms of $N = (A-1)$ Jacobi coordinates $\vec{\eta}_i$. One can write the wave function in terms of an HH expansion

$$\begin{aligned}\Phi(\vec{\eta}_1..&\vec{\eta}_{A-1}, s_1..s_A, t_1..t_A) = \sum_{K\nu} R_{K\nu}(\rho) H_{K\nu}(\Omega, s_1..s_A, t_1..t_A) \\ &\equiv \sum_{K\nu} \Phi_{K\nu}(\vec{\eta}_i, s_1..s_A, t_1..t_A),\end{aligned}\quad (1)$$

where, in case of nucleons,

$$\begin{aligned}H_{K\nu}(\Omega, s_1..s_A, t_1..t_A) = \sum_{Y_{A-1}} \frac{\Lambda_{\Gamma_A, Y_{A-1}}}{\sqrt{|\Gamma_A|}} \mathcal{Y}_{K_N L_N M_N \Gamma_A Y_{A-1} \alpha_N^K}(\Omega) \times \\ \mathcal{X}_{SS^z TT^z \tilde{\Gamma}_A \tilde{Y}_{A-1} \alpha_A^{ST}}(s_1..s_A, t_1..t_A)\end{aligned}\quad (2)$$

represent the hyperspherical harmonic functions coupled to the spin-isospin basis functions to yield the totally antisymmetric wave function. The $\mathcal{Y}_{K_N L_N M_N \Gamma_A Y_{A-1} \alpha_N^K}(\Omega)$ are the so called symmetrized hyperspherical functions that depend on the N Jacobi coordinates. They are HH functions with hyperspherical angular momentum $K = K_N$, and good angular momentum quantum numbers L_N, M_N that belong to well defined irreducible representations (irreps) $\Gamma_1 \in \Gamma_2 \dots \in \Gamma_A$, of the permutation group-subgroup chain $\mathcal{S}_1 \subset \mathcal{S}_2 \dots \subset \mathcal{S}_A$, denoted by the Yamanouchi symbol $[\Gamma_A, Y_{A-1}] \equiv [\Gamma_A, \Gamma_{A-1}, \dots, \Gamma_1]$. The dimension of the irrep Γ_n is denoted by $|\Gamma_n|$ and $\Lambda_{\Gamma_A, Y_{A-1}}$ is a phase factor [8]. Similarly, the function $\mathcal{X}_{SS^z TT^z \tilde{\Gamma}_A \tilde{Y}_{A-1} \alpha_A^{ST}}$ is a symmetrized spin-isospin state with good quantum numbers S, S^z, T and T^z . The label α_N^K (α_A^{ST}) is needed to remove the degeneracy of the hyperspherical (spin-isospin) states with a given symmetry. The argument of the hyperradial function $R_{K\nu}$ is the hyperradius ρ defined by

$$\rho^2 = \sum_i \eta_i^2, \quad (3)$$

Ω is the (3A-4)-dimensional hyperangle, and for brevity we shall use ν for all the quantum numbers but K , i.e. $\nu \equiv (L_N M_N SS^z TT^z \Gamma_A \alpha_N^K \alpha_A^{ST})$. In what follows we shall use the subscript N to denote A particle quantum numbers that depend on the Jacobi coordinates, and the subscript $A - 1$ for the $A - 1$ particle subsystem.

It is well known that finding a solution of the Schrödinger equation in terms of the ansatz (1) can be very difficult because the number of basis functions increases very fast with K and in order to have a real convergence one must use a huge number of basis functions [9]. Therefore a correlation function is advantageous to give the wave function a proper behavior [10]. Its advantages have been extensively verified for classical few-body systems reaching a high level of accuracy [11,12]. A general ansatz within the two-body correlation scheme is the Jastrow factor

$$\Psi = \prod_{i < j} f_{ij} \Phi, \quad (4)$$

where f_{ij} is a two-body correlation function. However, the use of the Jastrow ansatz leads to $3A - 3$ dimensional integrals. Therefore it is more convenient to use the so called pair correlation ansatz

$$\Psi = \sum_{i < j} \chi_{ij} \Phi, \quad (5)$$

because in this case one can use the Faddeev approach which leads to at most four–body integrals. In the Faddeev approach the Schrödinger equation is replaced by equivalent equations,

$$(T - E) \Psi_{ij} = -V_{ij} \Psi, \quad (6)$$

where $\Psi = \sum_{i < j} \Psi_{ij}$. In order to speed up the convergence these equations can be further modified [4] to include the contribution of the hypercentral potential explicitly. The hypercentral potential $V_{hc}(\rho)$ is defined as the projection of the two–body interaction on the subspace of the lowest order hyperspherical state, i.e. the hyperspherical state expressed in Eq. (2), with the minimal K :

$$V_{hc}(\rho) = \int d\Omega H_{K_{min}\nu}^\dagger(\Omega, s_i, t_i) V(\vec{r}_{1,2}, s_1, s_2, t_1, t_2) H_{K_{min}\nu}(\Omega, s_j, t_j). \quad (7)$$

Here the integration is carried over the $3N - 1$ dimensional hypersphere, and an implicit summation over all the spin–isospin states is understood. With the help of this definition we can rewrite Eq. (6) as follows

$$\left[T + \frac{A(A-1)}{2} V_{hc}(\rho) - E \right] \Psi_{ij} = -[V_{ij} - V_{hc}(\rho)] \Psi. \quad (8)$$

Motivated by the pair–correlation ansatz (5) we shall expand the Faddeev amplitude Ψ_{ij} in the following way,

$$\Psi_{ij} = \sum_p \Phi_p(\rho, \Omega) \chi_p(z_{ij}) = \sum_{K\nu p} R_{K\nu p}(\rho) H_{K\nu}(\Omega, s_1..s_A, t_1..t_A) \chi_p(z_{ij}), \quad (9)$$

where $\chi_p(z_{ij})$ is a polynomial of order p , and z_{ij} is related to the relative two–body distance through

$$z_{ij} = r_{ij}/\rho. \quad (10)$$

Although expanding the correlation function in terms of z_{ij} should be equivalent to an expansion in r_{ij} , it is more stable numerically to take $\chi_p(z_{ij})$ since r_{ij} goes to zero with ρ . Substituting the expansion of Eq. (9) into Eq. (6) we get

$$\left[-\frac{1}{2} \sum_{n=1}^{A-1} \Delta_n + \frac{A(A-1)}{2} V_{hc}(\rho) - E \right] \sum_p \Phi_p \chi_p(z_{ij}) = -[V_{ij} - V_{hc}(\rho)] \sum_p \Phi_p \sum_{k>l} \chi_p(z_{kl}), \quad (11)$$

where Δ_n is the Laplace operator associated with the n ’th Jacobi coordinate $\vec{\eta}_n$. Multiplying Eq. (11) on the left by $(H_{K'\nu'} \chi_{p'}(z_{ij}))^\dagger$ and using the notation

$${}_{ij} \langle K'\nu' p' | \hat{O} | K\nu p \rangle_{kl} = \int d\Omega H_{K'\nu'}^\dagger(\Omega, s_n, t_n) \chi_{p'}^*(z_{ij}) \hat{O} H_{K\nu}(\Omega, s_m, t_m) \chi_p(z_{kl}) \quad (12)$$

we get

$$\begin{aligned} \sum_{K\nu p} ij < K' \nu' p' | - \frac{1}{2} \sum_{n=1}^{A-1} \Delta_n + \frac{A(A-1)}{2} V_{hc}(\rho) - E | K \nu p >_{ij} R_{K\nu p}(\rho) = \\ & - \sum_{K'' \nu'' p''} ij < K' \nu' p' | [V_{ij} - V_{hc}(\rho)] \sum_{k>l} | K'' \nu'' p'' >_{kl} R_{K'' \nu'' p''}(\rho) . \end{aligned} \quad (13)$$

If the norm matrix

$$A_{K' \nu' p', K \nu p} \equiv_{ij} < K' \nu' p' | K \nu p >_{ij} \quad (14)$$

is non singular, one can define the projection operator

$$\hat{Q} = \sum_{K \nu p, K' \nu' p'} | K' \nu' p' > A_{K' \nu' p', K \nu p}^{-1} < K \nu p | . \quad (15)$$

The projection operator commutes with V_{ij} and one can rewrite Eq. (13) in the following form

$$\begin{aligned} \sum_{K \nu p} ij < K' \nu' p' | - \frac{1}{2} \sum_{n=1}^{A-1} \Delta_n + \frac{A(A-1)}{2} V_{hc}(\rho) - E | K \nu p >_{ij} R_{K \nu p}(\rho) = \\ & - \sum_{K \nu p} \sum_{K'' \nu'' p''} \sum_{K''' \nu''' p'''} ij < K' \nu' p' | [V_{ij} - V_{hc}(\rho)] | K'' \nu'' p'' >_{ij} \times \\ & A_{K'' \nu'' p'', K''' \nu''' p'''}^{-1} \sum_{kl} ij < K''' \nu''' p''' | K \nu p >_{kl} R_{K \nu p}(\rho) . \end{aligned} \quad (16)$$

Using the hyperspherical coordinates, and the following definitions

$$\begin{aligned} T_{K' \nu' p', K \nu p} &= ij < K' \nu' p' | \hat{K} | K \nu p >_{ij} , \\ V_{K' \nu' p', K \nu p}^r(\rho) &= ij < K' \nu' p' | V_{ij} - V_{hc} | K \nu p >_{ij} , \\ W_{K' \nu' p', K \nu p}^{[3]} &= \sum_{K'' \nu'' p''} A_{K' \nu' p', K'' \nu'' p''}^{-1} ij < K'' \nu'' p'' | K \nu p >_{ik} , \quad k \neq i, j , \\ W_{K' \nu' p', K \nu p}^{[4]} &= \sum_{K'' \nu'' p''} A_{K' \nu' p', K'' \nu'' p''}^{-1} ij < K'' \nu'' p'' | K \nu p >_{kl} , \quad k, l \neq i, j , \end{aligned} \quad (17)$$

Eq. (16) can be expressed as an hyperradial equation

$$\begin{aligned} \sum_{\mu'} \left[-\frac{1}{2} A_{\mu\mu'} \left(\frac{d^2}{d\rho^2} + \frac{3A-4}{\rho} \frac{d}{d\rho} \right) + \frac{1}{2} \frac{T_{\mu\mu'}}{\rho^2} + \frac{A(A-1)}{2} V_{hc}(\rho) A_{\mu\mu'} - E A_{\mu\mu'} \right] R_{\mu'}(\rho) \\ = - \sum_{\mu' \mu''} V_{\mu\mu'}^r(\rho) \left(\delta_{\mu' \mu''} + 2(A-2) W_{\mu', \mu''}^{[3]} + \frac{(A-2)(A-3)}{2} W_{\mu', \mu''}^{[4]} \right) R_{\mu''}(\rho) . \end{aligned} \quad (18)$$

Here $\mu \equiv (K \nu p)$, and \hat{K} is the generalized, hyperspherical, angular momentum operator. This hyperradial equation can be solved by expanding the hyperradial function $R_\mu(\rho)$ into basis functions $\phi_{n_\rho}(\rho)$

$$R_\mu(\rho) = \sum_{n_\rho} C_{n_\rho}^\mu \phi_{n_\rho}(\rho) \quad (19)$$

containing the Laguerre polynomials $L_{n_\rho}^a$

$$\phi_{n_\rho}(\rho) = \sqrt{\frac{n_\rho!}{(n_\rho + a)!}} b^{\frac{-3(A-1)}{2}} \left(\frac{\rho}{b}\right)^{\frac{a-(3A-4)}{2}} L_{n_\rho}^a\left(\frac{\rho}{b}\right) \exp\left[-\frac{\rho}{2b}\right]. \quad (20)$$

Multiplying the right and left hand sides by $\phi_{n_\rho}^*(\rho)$ and performing the hyperradial integration one remains with the generalized eigenvalue problem

$$\sum_m C_m (\mathbf{H}_{mn} - E \mathbf{M}_{mn}) = 0, \quad (21)$$

where m and n stand for the sets K, ν, p, n_ρ and K', ν', p', n'_ρ , respectively, and the matrix elements \mathbf{H}_{mn} and \mathbf{M}_{mn} are given by the corresponding hyperradial integrals.

Eq. (18) represents the main equation of the present method. The following remarks have to be stressed in order here:

1. the 3(A-1)-dimensional Schrödinger equation has been reduced to a 3×4 dimensional integro-differential equation, due to the presence of at most four-body terms ($W_{K'\nu'K\nu}^{[4]}$);
2. to the extent the convergence in the expansions is reached the result for $\Psi = \sum_{i < j} \Psi_{ij}$ can be considered as an "exact" ground state solution of the many-body Schrödinger equation.

III. CONSTRUCTION OF THE BASIS FUNCTIONS

Technical difficulties in calculating the matrix elements \mathbf{H}_{mn} and \mathbf{M}_{mn} are encountered in the construction of the basis functions $H_{K\nu}(\Omega, s_i, t_i)$ for increasing numbers of particles and hyperspherical angular momentum K , as well as in the calculation of the two-, three- and four-body terms that appear in \mathbf{H}_{mn} and \mathbf{M}_{mn} . The basis functions $H_{K\nu}(\Omega, s_i, t_i)$ must be totally antisymmetric functions in total space (coordinate, spin, isospin). Therefore, one needs efficient algorithms to construct convenient expressions for the symmetrized spin-isospin basis functions as well as symmetrized hyperspherical wave functions.

A. Spin-isospin states with arbitrary permutational symmetry

The construction of A-particle symmetrized spin-isospin functions as well as hyperspherical functions can be done recursively [8]. Each A-particle spin-isospin function of a well defined irrep of the symmetric group Γ_A and spin-isospin quantum numbers S_A, T_A , is written as a linear combination of spin-isospin coupled products of an (A-1)-particle wave function of well defined irrep Γ_{A-1} and spin-isospin quantum numbers S_{A-1}, T_{A-1} , and the A'th particle wave function with spin-isospin quantum numbers s_A, t_A . The coefficients of this linear combination are a sort of coefficients of fractional parentage. The subspace of functions with good quantum numbers S_A, T_A and Γ_{A-1} is an invariant subspace for the transposition class-sum operator of the symmetric group \mathcal{S}_A . The eigenvalues that are obtained after the diagonalization of the class-sum operator identify the irreps of the symmetric group uniquely. The eigenvectors are the spin-isospin coefficients of fractional parentage (stcfps)

$$\begin{aligned} \mathcal{X}_{S_A S_{A'} T_A T_{A'} \Gamma_A Y_{A-1} \alpha_A^{ST}}(s_i t_i) = & \sum_{S_{A-1} T_{A-1} \alpha_{A-1}^{TS}} \\ & [(S_{A-1}; s_A) S_A(T_{A-1}; t_A) T_A \Gamma_{A-1} \alpha_{A-1}^{ST}] \{ S_A T_A \Gamma_A \alpha_A^{ST} \} \times \\ & [\mathcal{X}_{S_{A-1} S_{A-1} T_{A-1} T_{A-1} \Gamma_{A-1} Y_{A-2} \alpha_{A-1}^{ST}} \otimes s_A t_A]^{S_A S_{A'} T_A T_{A'}}. \end{aligned} \quad (22)$$

The sum over S_{A-1} and T_{A-1} in Eq. (22) is subject to the usual angular momentum coupling rules.

B. Symmetrized hyperspherical functions

In an analogous way, one can use the recursive methods developed in the last few years [13,14] for constructing hyperspherical functions that belong to well defined irreps of the symmetric group. In this methods the reduction problem $\mathcal{O}_{3A-3} \supset \mathcal{O}_3 \otimes \mathcal{S}_A$ is solved and one obtains hyperspherical functions which belong to irreps of the symmetric group \mathcal{S}_A and have good angular momentum and hyperspherical angular momentum quantum numbers. These functions are expressed in terms of \mathcal{S}_{A-1} hyperspherical states, that are coupled, via the “tree” method [15], with the appropriate single-Jacobi coordinate hyperspherical functions, into coupled A -particle states with the desired angular momentum and hyperspherical angular momentum quantum numbers. Actually, these coupled states yield an invariant subspace with respect to \mathcal{S}_A . The transposition class-sum of the symmetric group (the second Casimir operator) is diagonalized within this subspace. The eigenvalues that are obtained after the diagonalization identify the irreps of the symmetric group uniquely, and the eigenvectors are the hyperspherical coefficients of fractional parentage (hscfps).

Constructing basis functions in such a recursive way makes the evaluation of any two body operator easy, since only the matrix element of the two-body operator between the last two particles needs to be calculated. A further improvement in the efficiency of the algorithm can be reached if one uses reversed order Jacobi coordinates for the construction of the hyperspherical functions. Normally Jacobi coordinates are defined so that the first one is the relative distance between particles 1 and 2, while the last is the distance between the A 'th particle and the center of mass of the $A-1$ particle system. This implies that in order to calculate the matrix element of a two-body operator, depending typically on the interparticle distance between the A 'th and $(A-1)$ 'th particles (see Section IV), one needs to rotate the last two Jacobi coordinates by a proper angle so that one of them represents the interparticle distance. This can be done by using the Raynal Revai, the T-coefficients and the 6-j coefficients. Constructing the Jacobi coordinates in reverse order, would simplify the calculation of two- and three-body matrix elements as no further rotation is needed [14].

Recently an alternative way to construct the symmetrized hyperspherical functions has been proposed [7]. This method consists in introducing as an intermediate subgroup the orthogonal group of kinematic rotations \mathcal{O}_{A-1} , i.e. one uses the group chain $\mathcal{O}_{3A-3} \supset \mathcal{O}_3 \otimes \mathcal{O}_{A-1} \supset \mathcal{O}_3 \otimes \mathcal{S}_A$. The introduction of the kinematic group turns out to be of particular importance for increasing number of particles and for large values of K as it results in a significant reduction in the number of hscfps and in the computation time. Another benefit in using this method is the realization of kinematic rotations through the representation matrices of the group \mathcal{O}_{A-1} thus avoiding the use of the Raynal–Revai and

the T-coefficients in calculating matrix elements of two-body operators depending on the interparticle distance. In the present calculation we have adopted this procedure, even if it is less efficient than defining Jacobi coordinates in reversed order. The reason is that in this way one can easily extend the present method to solve the Schrödinger-like equation with source, necessary for the calculation of the Lorentz integral transforms of response functions [16]. The presence of the source annuls the advantages of the alternative set of Jacobi coordinates.

Summarizing the procedure for the construction of the symmetrized hyperspherical harmonics one can split it into two steps. In the first step one constructs hyperspherical functions with good orthogonal symmetry, i.e. basis functions with good quantum numbers K_N, L_N, M_N that belong to a well defined Gel'fand-Zetlin pattern $\Lambda_N = (\lambda_N, \lambda_{N-1}, \dots, \lambda_2)$. The orthogonal group irreps $\lambda_j, (j = 2, 3, \dots)$ are characterized by the integer or half integer numbers $\lambda_{j,1}, \lambda_{j,2}, \dots, \lambda_{j,k}$, where $k = [\frac{j}{2}]$. In Ref. [7] it was pointed out that for hyperspherical functions these numbers are always integers and, in addition, there are at most three non-zero values in the irrep λ_j for $j \geq 6$ i.e., $\lambda_{j,1}, \lambda_{j,2}$, and $\lambda_{j,3}$. The second step is to reduce each irrep of the orthogonal group \mathcal{O}_N into irreps of the symmetry group \mathcal{S}_{N+1} . These two steps are carried out using the recursive method developed in Ref. [7]. At the end, the symmetrized A-particle, N -Jacobi coordinate, hyperspherical states can be expressed in terms of $(A-1)$ -particle states coupled to the A 'th particle state by using two new types of coefficients of fractional parentage, namely the orthogonal-hyperspherical cfps (ohscfps) for the construction of hyperspherical functions with good orthogonal symmetry and the orthogonal cfps (ocfps) for the reduction $\mathcal{O}_{A-1} \downarrow \mathcal{S}_A$. One has

$$\begin{aligned} & \mathcal{Y}_{K_N L_N M_N} \lambda_N \beta_N^K \Gamma_A Y_{A-1} \beta_A^\lambda(\Omega) \\ &= \sum_{\lambda_{N-1} \beta_{A-1}^\lambda} [(\lambda_{N-1} \Gamma_{A-1} \beta_{A-1}^\lambda) \lambda_N | \} \lambda_N \Gamma_A \beta_A^\lambda] \times \\ & \quad \sum_{K_{N-1} L_{N-1} \beta_{N-1}^K \ell_N} [(K_{N-1} L_{N-1} \lambda_{N-1} \beta_{N-1}^K; \ell_N) K_N L_N | \} K_N L_N \lambda_N \beta_N^K] \\ & \quad \mathcal{Y}_{(K_{N-1} L_{N-1} \lambda_{N-1} \beta_{N-1}^K \Gamma_{A-1} Y_{A-2} \beta_{A-1}^\lambda; \ell_N) K_N L_N M_N}(\Omega) . \end{aligned} \quad (23)$$

Note that the order of the summation in this equation is important. We have to start from the sum over the ocfps

$$[(\lambda_{N-1} \Gamma_{A-1} \beta_{A-1}^\lambda) \lambda_N | \} \lambda_N \Gamma_A \beta_A^\lambda], \quad (24)$$

to determine the irrep λ_{N-1} of \mathcal{O}_{N-1} and then we can sum over the ohscfps

$$[(K_{N-1} L_{N-1} \lambda_{N-1} \beta_{N-1}^K; \ell_N) K_N L_N | \} K_N L_N \lambda_N \beta_N^K], \quad (25)$$

where $(\beta_N^K$ and $\beta_A^\lambda)$ are the degeneracy removing labels $((\beta_N^K, \beta_A^\lambda) \equiv \alpha_N^K)$.

IV. CALCULATION OF THE MATRIX ELEMENTS

The matrix elements of any two-body operator

$$O_{ij} = O^R(\vec{r}_{ij})O^{ST}(s_i, s_j, t_i, t_j) \quad (26)$$

between the fermionic, antisymmetric, hyperspherical basis functions of Eq. (2), can be written as a sum of a spatial term multiplied by a spin-isospin term,

$$\begin{aligned} < K\nu | O_{ij} | K'\nu' > &= \sum_{\Gamma_{A-1}\Gamma'_{A-1}\Gamma_{A-2}} \prod(\text{ISF}) \times \\ &< S_A S^z A T_A T'^z_A \tilde{\Gamma}_A \tilde{Y}_{A-1} \alpha_A^{ST} | O^{ST}(s_i, s_j, t_i, t_j) | S'_A S'^z_A T'_A T'^z_A \tilde{\Gamma}'_A \tilde{Y}'_{A-1} \alpha'^{ST}_A > \times \\ &< K_N L_N M_N \boldsymbol{\lambda}_N \beta_N^K \Gamma_A Y_{A-1} \beta_A^\lambda | O^R(\vec{r}_{ij}) | K'_N L'_N M'_N \boldsymbol{\lambda}'_N \beta'_N^K \Gamma'_A Y'_{A-1} \beta'_A^\lambda >, \end{aligned} \quad (27)$$

where the sum runs over all the $\mathcal{S}_{A-2}, \mathcal{S}_{A-1}$ irreps $\Gamma_{A-1}\Gamma'_{A-1}\Gamma_{A-2}$ such that $\Gamma_{A-2} \in \Gamma_{A-1} \in \Gamma_A$ and $\Gamma_{A-2} \in \Gamma'_{A-1} \in \Gamma'_A$. The factor preceding the spatial and spin-isospin matrix element is a product of the inner product symmetric group isoscalar factors for the antisymmetric representation and is given by

$$\prod(\text{ISF}) = \Lambda_{\Gamma_A \Gamma_{A-1}} \sqrt{\frac{|\Gamma_{A-1}|}{|\Gamma_A|}} \Lambda_{\Gamma_{A-1} \Gamma_{A-2}} \sqrt{\frac{|\Gamma_{A-2}|}{|\Gamma_{A-1}|}} \Lambda_{\Gamma'_A \Gamma'_{A-1}} \sqrt{\frac{|\Gamma'_{A-1}|}{|\Gamma'_A|}} \Lambda_{\Gamma'_{A-1} \Gamma'_{A-2}} \sqrt{\frac{|\Gamma'_{A-2}|}{|\Gamma'_{A-1}|}}. \quad (28)$$

The phase factor $\Lambda_{\Gamma_A \Gamma_{A-1}}$ [17] is positive (negative) when the number of boxes in Γ_A below the row of the A 'th particle is even (odd).

Using the permutation symmetry of the HH states the matrix elements of any two-body operator, O_{ij} , are equal to the matrix elements of $O_{A,A-1}$. The spatial matrix elements are then calculated using the last two generations of cfps, referring to the constructions $A-2 \rightarrow A-1$ and $A-1 \rightarrow A$, and the appropriate kinematical rotations which reduce the calculation of any two-body operator to sum over one dimensional integrals. The formal derivation of the calculation of two-body operator matrix elements between the symmetrized hyperspherical harmonics of Eq. (23) has been presented in rather a detailed manner by Barnea and Novoselsky [18]. Summarizing their results one has

$$\begin{aligned} < K_N L_N M_N \boldsymbol{\lambda}_N \beta_N^K \Gamma_A Y_{A-1} \beta_A^\lambda | O^R(\vec{r}_{A,A-1}) | K'_N L'_N M'_N \boldsymbol{\lambda}'_N \beta'_N^K \Gamma'_A Y'_{A-1} \beta'_A^\lambda > = \\ &\delta_{\Gamma_{A-2}, \Gamma'_{A-2}} \sum_{\boldsymbol{\lambda}_{N-1} \beta_{A-1}^\lambda} \sum_{\boldsymbol{\lambda}'_{N-1} \beta_{A-1}^{\lambda'}} \sum_{\boldsymbol{\lambda}_{N-2} \beta_{A-2}^\lambda} \\ &[(\boldsymbol{\lambda}_{N-1} \Gamma_{A-1} \beta_{A-1}^\lambda) \boldsymbol{\lambda}_N |] \boldsymbol{\lambda}_N \Gamma_A \beta_A^\lambda [* [(\boldsymbol{\lambda}'_{N-1} \Gamma'_{A-1} \beta_{A-1}^{\lambda'}) \boldsymbol{\lambda}'_N |] \boldsymbol{\lambda}'_N \Gamma'_A \beta'_A^{\lambda'}] \\ &\times [(\boldsymbol{\lambda}_{N-2} \Gamma_{A-2} \beta_{A-2}^\lambda) \boldsymbol{\lambda}_{N-1} |] \boldsymbol{\lambda}_{N-1} \Gamma_{A-1} \beta_{A-1}^{\lambda'} [* [(\boldsymbol{\lambda}_{N-2} \Gamma_{A-2} \beta_{A-2}^\lambda) \boldsymbol{\lambda}'_{N-1} |] \boldsymbol{\lambda}'_{N-1} \Gamma'_{A-1} \beta'_{A-1}^{\lambda'}] \\ &\times \sum_{\boldsymbol{\lambda}''_{N-1}} D \frac{\boldsymbol{\lambda}_N^*}{\boldsymbol{\lambda}''_{N-1} \tilde{\boldsymbol{\Lambda}}_{N-1}} (g_{A,A-1}) D \frac{\boldsymbol{\lambda}'_N}{\boldsymbol{\lambda}''_{N-1} \tilde{\boldsymbol{\Lambda}}'_{N-1}} (g_{A,A-1}) \\ &\times < K_N L_N M_N \boldsymbol{\lambda}_N \beta_N^K \tilde{\boldsymbol{\Lambda}}''_{N-1} Y_{A-2} \beta_{A-2}^\lambda | O^R(\sqrt{2}\vec{\xi}_N) | K'_N L'_N M'_N \boldsymbol{\lambda}'_N \beta'_N^K \tilde{\boldsymbol{\Lambda}}''_{N-1} Y_{A-2} \beta'_A^\lambda >. \end{aligned} \quad (29)$$

Here, for simplicity, we use the symbol $\boldsymbol{\Lambda}_{N-1}$ to denote the irreps $[\boldsymbol{\lambda}_{N-1}, \boldsymbol{\lambda}_{N-2}]$. Note that the sum in Eq. (29) over the irreps $\boldsymbol{\lambda}''_{N-1}$ is restricted to those states which belong both to the irrep $\boldsymbol{\lambda}_N$ and $\boldsymbol{\lambda}'_N$. The kinematical “relative coordinate” rotation applied to the Jacobi coordinates

$$\begin{aligned} \vec{\xi}_{N-1} &= \sqrt{\frac{2(A-2)}{A}} \left(\frac{\vec{r}_{A-1} + \vec{r}_A}{2} - \frac{1}{A-2} \sum_{i=1}^{A-2} \vec{r}_i \right) \\ \vec{\xi}_N &= \sqrt{\frac{1}{2}} (\vec{r}_A - \vec{r}_{A-1}), \end{aligned} \quad (30)$$

and given by

$$\begin{aligned}\vec{\xi}_{N-1} &= \sqrt{\frac{A}{2(A-1)}}\vec{\eta}_{N-1} + \sqrt{\frac{A-2}{2(A-1)}}\vec{\eta}_N \\ \vec{\xi}_N &= -\sqrt{\frac{A-2}{2(A-1)}}\vec{\eta}_{N-1} + \sqrt{\frac{A}{2(A-1)}}\vec{\eta}_N ,\end{aligned}\quad (31)$$

is realized in Eq. (29) by the generalized, \mathcal{O}_N , Wigner D functions, where $g_{A,A-1}$ is the group element that corresponds to the rotation (31), i.e. a rotation by an angle $\gamma = \arcsin(\sqrt{\frac{A-2}{2(A-1)}})$ in the $\vec{\eta}_N, \vec{\eta}_{N-1}$ plane.

Since the two-body operator in Eq. (29) depends only on the coordinate $\vec{\xi}_N$ we should separate the hyperspherical functions related to this coordinate in the bra and the ket states. So, the last step in the derivation consists of using the ohscfps introduced in Eq. (25). Then, the last term on the rhs of Eq. (29) is

$$\begin{aligned}< K_N L_N M_N \boldsymbol{\lambda}_N \beta_N^K \tilde{\Lambda}_{N-1}'' Y_{A-2} \beta_{A-2}^\lambda | O^R(\sqrt{2}\vec{\xi}_N) | K'_N L'_N M'_N \boldsymbol{\lambda}'_N \beta_N^{K'} \tilde{\Lambda}_{N-1}'' Y_{A-2} \beta_{A-2}^{\lambda'} > = \\ \sum_{K_{N-1} L_{N-1} \beta_{N-1}^K \ell_N, \ell'_N} &\left[(K_{N-1} L_{N-1} \boldsymbol{\lambda}_{N-1} \beta_{N-1}^K; \ell_N) K_N L_N | \right] K_N L_N \boldsymbol{\lambda}_N \beta_N^K \\ &\times \left[(K_{N-1} L_{N-1} \boldsymbol{\lambda}_{N-1} \beta_{N-1}^K; \ell'_N) K'_N L'_N | \right] K'_N L'_N \boldsymbol{\lambda}'_N \beta_N^{K'} \\ &\times < (K_{N-1} L_{N-1} \dots; \ell_N) K_N L_N M_N | O^R(\sqrt{2}\vec{\xi}_N) | (K_{N-1} L_{N-1} \dots; \ell'_N) K'_N L'_N M'_N > .\end{aligned}\quad (32)$$

This matrix element can be calculated for any given two-body operator. For scalar operator $O^R(r_{A,A-1})$, one obtains

$$\begin{aligned}O_{K_N K'_N; K_{N-1} \ell_N}^R(\rho) &\equiv \\ < (K_{N-1} L_{N-1} \dots; \ell_N) K_N L_N M_N | O^R(\sqrt{2}\vec{\xi}_N) | (K_{N-1} L_{N-1} \dots; \ell'_N) K'_N L'_N M'_N > = \\ \delta_{\ell_N, \ell'_N} \mathcal{N}_N(K_N; \ell_N K_{N-1}) \mathcal{N}_N(K'_N; \ell_N K_{N-1}) &\int_0^{\frac{\pi}{2}} d\theta \sin^{2\ell_N+2}(\theta) \cos^{2K_{N-1}+3N-4}(\theta) \\ &\times P_n^{(\ell_N+\frac{1}{2}, K_{N-1}+\frac{3N-5}{2})}(\cos 2\theta) P_{n'}^{(\ell_N+\frac{1}{2}, K_{N-1}+\frac{3N-5}{2})}(\cos 2\theta) O^R(\sqrt{2}\rho \sin \theta) ,\end{aligned}\quad (33)$$

with $n = \frac{K_N - \ell_N - K_{N-1}}{2}$, $n' = \frac{K'_N - \ell_N - K_{N-1}}{2}$ and where

$$\mathcal{N}_N(K_N; \ell_N K_{N-1}) = \left[\frac{(2K_N + 3N - 2)n! \Gamma(n + K_{N-1} + \ell_N + \frac{3N-2}{2})}{\Gamma(n + \ell_N + \frac{3}{2}) \Gamma(n + K_{N-1} + \frac{3N-3}{2})} \right]^{\frac{1}{2}} \quad (34)$$

is a normalization constant, and $P_n^{(a,b)}$ are the Jacobi polynomials.

The spin-isospin part of the two-body operator is calculated in a similar way, first we use the last two generations of the spin-isospin cfps (Eq. (22)) to get the explicit dependence of the state $|S_A S^z_A T_A T^z_A \tilde{\Gamma}_A \tilde{Y}_{A-1} \alpha_A^{ST}|$ on the spin and the isospin of the last two-particles,

$$\begin{aligned}< S_A S^z_A T_A T^z_A \Gamma_A Y_{A-1} \alpha_A^{ST} | O^{ST}(s_A, s_{A-1}, t_A, t_{A-1}) | S'_A S'^z_A T'_A T'^z_A \Gamma'_A Y'_{A-1} \alpha'^{ST}_A > = \\ \delta_{Y_{A-2}, Y'_{A-2}} \sum_{S_{A-1} T_{A-1} \alpha_{A-1}^{ST}} \sum_{S'_{A-1} T'_{A-1} \alpha'^{ST}_{A-1}} &[(S_{A-1}; s_A) S_A(T_{A-1}; t_A) T_A \Gamma_{A-1} \alpha_{A-1}^{ST} | \} S_A T_A \Gamma_A \alpha_A^{ST}] \\ &\times [(S'_{A-1}; s_A) S'_A(T'_{A-1}; t_A) T'_A \Gamma'_A \alpha'^{ST}_{A-1} | \} S'_A T'_A \Gamma'_A \alpha'^{ST}_A]\end{aligned}$$

$$\begin{aligned}
& \times \sum_{S_{A-2}T_{A-2}\alpha_{A-2}^{ST}} [(S_{A-2}; s_A) S_{A-1}(T_{A-2}; t_A) T_{A-1}\Gamma_{A-2}\alpha_{A-2}^{ST}] \{ S_{A-1}T_{A-1}\Gamma_{A-1}\alpha_{A-1}^{ST} \\
& \times [(S_{A-2}; s_A) S'_{A-1}(T_{A-2}; t_A) T'_{A-1}\Gamma_{A-2}\alpha_{A-2}^{ST}] \{ S'_{A-1}T'_{A-1}\Gamma'_{A-1}\alpha'_{A-1}^{ST} \} \\
& \times < S_A T_A S_{A-1} T_{A-1} S_{A-2} T_{A-2} \dots | O^{ST}(s_A, s_{A-1}, t_A, t_{A-1}) | S'_A T'_A S'_{A-1} T'_{A-1} S'_{A-2} T'_{A-2} \dots > .
\end{aligned} \tag{35}$$

Then the matrix element on the rhs of (35) is calculated using the $6j$ symbols.

Special attention should be payed to the matrix elements of the generalized angular momentum operator \hat{K} as it contains the hyperangular part of the Laplace operator. Using the definition in Eq. (12) we see that

$$T_{K'\nu'p',K\nu p} = < K'\nu' | \chi_{p'}(z_{ij})^* \hat{K} \chi_p(z_{ij}) | K\nu > . \tag{36}$$

This matrix element can be easily calculated once we know the action of \hat{K} on $\chi_p(z_{ij})$. Since \hat{K} is invariant under kinematical rotations we can always write it using a set of Jacobi coordinates such that $\vec{\xi}_N = \frac{1}{\sqrt{2}}(\vec{r}_i - \vec{r}_j)$, which leads to the following expression

$$\begin{aligned}
& < K'\nu' | \chi_{p'}(z_{ij})^* \hat{K} \chi_p(z_{ij}) | K\nu > = \\
& < K'\nu' | \chi_{p'}(z_{ij})^* K(K + 3N - 2) \chi_p(z_{ij}) - \chi_{p'}(z_{ij})^* (1 - z_{ij}^2) \frac{d^2 \chi_p(z_{ij})}{dz_{ij}^2} \\
& + \chi_{p'}(z_{ij})^* \left\{ z_{ij} + \frac{-2 + (3N - 2)z_{ij}^2}{z_{ij}} \right\} \frac{d \chi_p(z_{ij})}{dz_{ij}} \\
& - 2\chi_{p'}(z_{ij})^* (1 - z_{ij}^2) \frac{d \chi_p(z_{ij})}{dz_{ij}} \frac{d}{dz_{ij}} | K\nu > .
\end{aligned} \tag{37}$$

This is just the matrix element of a sum of two body operators which can be calculated as explained above.

A bit more problematic are the three- and four-body integrals $W_{K'\nu'p'K\nu p}^{[3]}$ and $W_{K'\nu'p'K\nu p}^{[4]}$. In order to calculate the three- (four-) body term we must first use three (four) generations of the ocfps in order to express the matrix elements in terms of the orthogonal symmetry adapted hyperspherical functions. Then we can use the proper rotations and reduce the integrals to six-dimensional integrals that depend only on the last two Jacobi coordinates. The explicit dependence of the HH functions on the Jacobi coordinates is then revealed using the last two generations of the ohscfps, Eq. (25). For $L = 0$ states, these integrals can further be reduced to three-dimensional integrations.

V. DISCUSSION OF THE RESULTS

The present method becomes more and more complex as the number of fermions increases. Therefore in this work we consider only central NN potentials. We present results for 6, 8 and 12 nucleons interacting via the Volkov [19] (VV), the Afnan–Tang [20] (S3), the modified S3 potential [21] (MS3), the Brink–Boeker [22] (B1) and the Malfliet–Tjon [23] potentials (MT–I/III and MT–V). The accuracy and convergence of the method have been investigated for 6 and 8 nucleons.

The first step in our numerical study was to determine the hyperradial working point, i.e. the parameters a and b of the Laguerre polynomials in Eq. (20), the number of radial

grid points and their location. After some preliminary tests we decided to use 15 hyperradial grid points and 15 hyperradial functions with the parameters $b = 0.25$ fm and $a = 12$. The grid points where chosen as the abscissas for a Gauss–Laguerre integration.

The next step in setting our working point was to check the convergence of the two–body correlation terms. As an example we studied the ${}^8\text{Be}$ system with the hard core MT–V potential, using a single HH function, with $K = 4$ and expanding the correlation function into Jacobi polynomials. As can be seen from Fig. 1 the binding energy converges very fast with increasing number n_x of polynomials . In fact, the energy difference between the calculations with 7 and 8 correlations terms is about 0.02 MeV. As a consequence we used 8 terms in the expansion of the correlation function.

The effect of introducing the hypercentral potential $V_{hc}(\rho)$ is presented in Table I for ${}^6\text{Li}$ with the VV potential. As can be seen the hypercentral potential accelerates the convergence of the HH expansion. With the lowest K_{max} of 2 one already obtains a larger binding energy than with $K_{max} = 6$ without hypercentral potential. Thus the introduction of V_{hc} is certainly advantageous.

Our numerical results with the parameters described above are presented in Table II for the 6 nucleon system and in Table III for the 8 nucleon system.

For ${}^6\text{Li}$ the calculations include only one line irreps of the kinematical group \mathcal{O}_5 and the irreps [42] and [33] of the permutation group. We compare our values with recent accurate variational results [2] available for some of these central potentials. One can notice that with the VV potential one reaches convergence faster than with other potentials. The result for the binding energy starts oscillating around the asymptotic value. It also compares nicely to the variational result of Ref. [2]. The other potentials show a tendency to convergence even if K_{max} is not large enough to reach it. The MT potentials seem to lead to a more rapid convergence than S3 and B1. The differences may be due both to the fact that the convergent value has not yet been reached and to the missing irreps of the permutation group. The two line irreps of the orthogonal group are of little importance. This has been checked for the 8 particle case, where they give rather small contributions.

The calculations for ${}^8\text{Be}$ include only the irrep (400) of the kinematical group \mathcal{O}_7 and irreps with at most 3 rows of the permutation group. Here the comparison is made with the TICI results [6]. In all cases our results for the binding energy are somewhat larger. They show characteristics similar to the six–body case. Again one sees that the VV potential result presents small oscillations around the convergent value and that the rather hard core MT potentials seem to give values closer to convergence than B1 or S3. From the comparison between the TICI results with and without state dependent correlations one can infer that for the MT potentials state independent correlations already give rather satisfying results, while state dependent correlations are more effective for B1 and S3. Since our correlations are state independent one could expect such a different convergence behavior as found in Table III

The results for ${}^{12}\text{C}$ are presented in Table IV. Here the calculations include a single HH state, $K_{max} = 8$, with the kinematical group \mathcal{O}_{11} irrep (4, 4, 0) and the \mathcal{S}_{12} irrep [444]. The comparison is made with TICI [6], IDEA [4], and the variational result of Ref. [24]. Again from the comparison with the TICI results one can see that S3 and B1 results are farer from convergence than the MT values and that state dependent correlations play a similar role as discussed for the ${}^8\text{Be}$ case.

The IDEA results for 12 particles deviate somewhat from ours, although they are all obtained using a single HH state. One possible explanation of the difference can be attributed to the choice of the HH state which is not unique. On the other hand we have obtained excellent agreement with the IDEA results for 16 bosons.

VI. CONCLUSIONS

In this work we have formulated a general method to calculate the wave functions of light systems up to considerably large number of particle. This method combines the main ideas of the HH expansion, the pair correlation ansatz and the Faddeev approach. The actual application of it is made possible by the use of a very efficient recursive algorithm to construct the antisymmetric A-particle state containing hyperspherical harmonics. We have applied the method to calculate the binding energies of 6, 8 and 12 nucleon systems with central local potentials. The results we have obtained are very encouraging. For some potentials (VV, 6 particles and MTV, 8 particles) we have reached the convergence region with $K_{max} = 8$ which is the maximum value allowed by our present computer facilities (workstations). The ${}^6\text{Li}$ result for the VV potential is slightly higher than the SVM result. Even if in other cases we have not yet reached the convergence in the HH expansion our results are close to the TICI results. For the eight-body case they are higher for all the potentials where results were available for a comparison.

The method presented here for the solution of the few-body Schrödinger equation can be easily extended to solve the Schrödinger-like equation with a source, necessary for the application of the Lorentz integral transform method. Work in this direction is in progress.

TABLES

TABLE I.

The effect of the hypercentral potential V_{hc} on the binding energy of six-nucleon system 6Li , $(L, S)J^\pi = (0, 1)1^+$, interacting via the VV potential.

K_{max}	$V_{hc} = 0$	$V_{hc} = \int d\Omega H_{K_{min}\nu}^\dagger V_{1,2} H_{K_{min}\nu}$
2	64.18	66.10
4	64.81	66.53
6	65.47	66.63

TABLE II.

Binding energies of six-nucleon system 6Li , $(L, S)J^\pi = (0, 1)1^+$, interacting via various NN potentials. N_{HH} represents the number of hyperspherical harmonic states.

K_{max}	N_{HH}	B1	MT-I/III	MTV	S3	VV
2	1	30.99	30.15	62.45	62.76	66.10
4	4	37.82	34.67	63.27	64.45	66.53
6	12	39.11	35.43	64.10	66.49	66.63
8	31	39.61	35.91	64.55	67.18	66.57
SVM [2]	-	-	-	66.30	70.65	66.25

TABLE III.

Binding energies of eight-nucleon system 8Be , $(L, S)J^\pi = (0, 0)0^+$, interacting via various NN potentials. Also given are results from Ref. [6] with state independent TICI_{SI} and state dependent TICI_{SD} correlations.

K_{max}	N_{HH}	B1	MT-I/III	MTV	S3	VV
4	1	56.71	52.82	134.29	31.19	147.42
6	4	65.39	59.31	137.72	38.08	148.70
8	15	70.03	60.64	137.80	42.11	148.49
TICI _{SI}		49.18	46.67	129.25	26.26	
TICI _{SD}		61.30	52.67	130.23	37.30	

TABLE IV.

Binding energy of twelve nucleon system ^{12}C , $(L, S)J^\pi = (0, 0)0^+$, interacting via various NN potentials. Also given are results from Refs. [6] (TICI), [4] (IDEA) and [24] (VMC). The TICI results as in Table III.

	B1	MT-I/III	MTV	S3	VV
This work	96.64	108.34	437.25	52.42	494.00
TICI	103.93	109.04	429.44	62.99	
IDEA	80.1			44.4	
VMC	82.9 ± 0.2				

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FIGURES

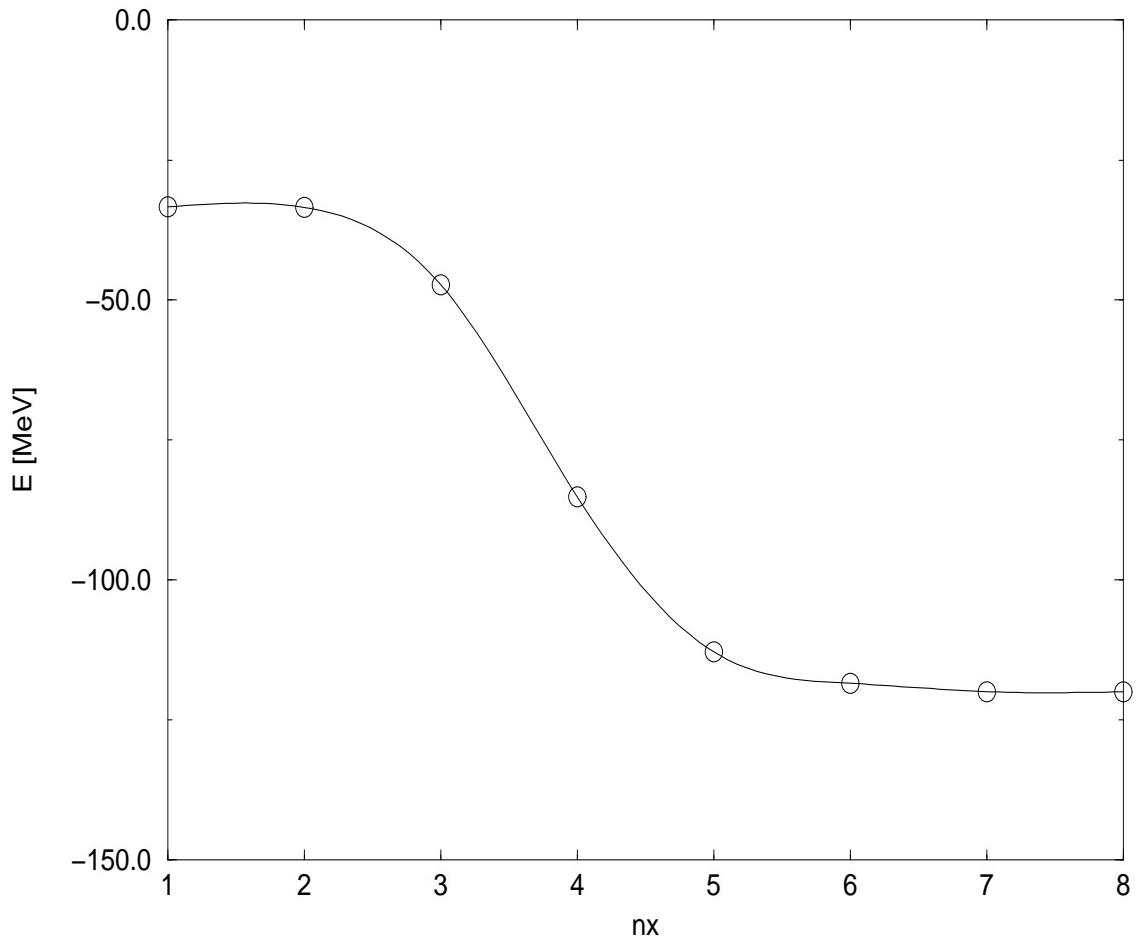


FIG. 1. Convergence of the binding energy with the number n_x of polynomials in the expansion of the correlation function. Results are presented for $A = 8$ and MTV potential.